Properties of Geometric Potential in the Invariant Adiabatic Theory

Mei-sheng Zhao[1*] and Jian-da Wu[1], Jian-lan Chen[1] and Yong-de Zhang[2]
[1] *Hefei National Laboratory for Physical Sciences at Microscale and Department of Modern Physics, University of Science and Technology of China, Hefei 230026, People's Republic of China.*
[2] *CCAST (World Laboratory), P.O. Box 8730, Beijing 100080, People's Republic of China*
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We concentrate on the geometric potential in the invariant perturbation theory of quantum adiabatic process which is presented in our recent papers. It is found out to be related to the geodesic curvature of the spherical curve in 2-dimension quantum systems. We also show that the geometric potential may affect adiabatic approximation remarkably.

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The Quantum Adiabatic Theorem is one of the most interesting conclusions in quantum theory [1, 2, 3, 4, 5, 6, 7]. It asserts that if the Hamiltonian of a time-dependent system varies infinitely slowly, then the system would always remain in the state possessing the same value of a certain dimensionless quantum number set as the initial state. Of course, *varies infinitely slow* is only a mathematical limitation. Denote the instantaneous eigenstates of a non-degenerate time-dependent quantum system as $\{|k\rangle,\ k=1,2,\cdots\}$ with corresponding instantaneous eigenvalues $\{E_k,\ k=1,2,\cdots\}$, the traditional quantum adiabatic approximation condition may be expressed as follows

$$\frac{|\langle m|\dot{n}\rangle|}{|E_m-E_n|}\ll 1, \tag{1}$$

the dot here and below expresses the derivative with respect to time. The validity of this condition had never been doubted until recent years[8, 9]. They pointed out that the validity of the traditional adiabatic approximation condition can not guarantee the validity of adiabatic approximation. Many efforts have been made to obtain new sufficient criterions of the adiabatic approximation[10, 11, 12, 13, 14, 15]. But none of them achieves a complete success because the conditions given by them are either too complicated or much more rigorous than necessary, therefore, are inconvenient to use. Nowadays with the development of the technique, more and more artificial micro-structures and controllable quantum systems appears, so time-dependent quantum systems are more and more important and quantum adiabatic approximation is more and more interesting. In our recent papers[16, 17] we present an invariant perturbation theory of quantum adiabatic proccess and proposed a new adiabatic approximation condition according to the invariance under time-dependent *U(1)* transformation. In this paper we will continue to study the physical and geometric meanings of the geometric potential in our adiabatic condition.

Consider a general d-dimension time-dependent quantum system, let us denote its Hamiltonian as $H(\tau),\ \tau\in\{0,T\}$. The instantaneous eigenstates of the Hamiltonian are $\{|k(\tau)\rangle, k=1,2,\cdots,d\}$, with corresponding energy eigenvalue $E_k(\tau), k=1,2,\cdots,d\}$. Denote $\gamma_{nm}(\tau)\equiv i\langle n(\tau)|\dot{m}(\tau)\rangle$, we can construct the *U(1) invariant adiabatic basis* [16, 17]

$$|\Phi_n^{adi}\rangle = e^{-i\int_0^\tau E_n(\lambda)d\lambda+i\int_0^\tau \gamma_{nn}(\lambda)d\lambda}|n(\tau)\rangle. \tag{2}$$

We have derived an adiabatic approximation condition[16]

$$\left|\frac{d}{d\tau}\arg\langle\Phi_n^{adia}(\tau)|\dot{\Phi}_m^{adia}(\tau)\rangle\right| \gg \left|\langle\Phi_n^{adia}(\tau)|\dot{\Phi}_m^{adia}(\tau)\rangle\right| \quad (\forall n\neq m), \tag{3}$$

which can be rewritten as follows

$$\left|E_n(\tau)-E_m(\tau)+\gamma_{mm}(\tau)-\gamma_{nn}(\tau)+\frac{d}{d\tau}\arg\gamma_{nm}(\tau)\right| \gg |\gamma_{nm}(\tau)| \quad (\forall\ n\neq m). \tag{4}$$

Compared with the traditional adiabatic approximation condition, the new condition Eq.(4) has one extra term

$$\begin{aligned}\Delta_{mn} &\equiv \gamma_{mm}(\tau)-\gamma_{nn}(\tau)+\frac{d}{d\tau}\arg\gamma_{nm}(\tau)\\ &= i\left(\langle m|\dot{m}\rangle-\langle n|\dot{n}\rangle\right)+\frac{d}{d\tau}\arg\langle n|\dot{m}\rangle,\end{aligned} \tag{5}$$

which is referred to as *quantum geometric potential*[16, 17].

We have revealed the invariance of this Geometric Potential under time-dependent *U(1)* transformation in [16]. Here we will show the relation between the geometric potential and the geodesic curvature of spherical curve in 2-dimension time-dependent quantum systems. Generally, we can write the Hamiltonian of a 2-dimension system as $H(\tau) = A(\tau)+B(\tau)\vec{n}(\tau)\cdot\vec{\sigma}$, where $\vec{n}(\tau) = (\sin\theta(\tau)\cos\varphi(\tau),\sin\theta(\tau)\sin\varphi(\tau),\cos\theta(\tau))$. Choosing appropriate phases, the Hamiltonian's instantaneous eigenstates or *adiabatic orbits* read

$$\begin{cases}|+,\tau\rangle = \cos\frac{\theta(\tau)}{2}|0\rangle+e^{i\varphi(\tau)}\sin\frac{\theta(\tau)}{2}|1\rangle\\ |-,\tau\rangle = \sin\frac{\theta(\tau)}{2}|0\rangle-e^{i\varphi(\tau)}\cos\frac{\theta(\tau)}{2}|1\rangle\end{cases}. \tag{6}$$

It's quite clear that polarization vectors of the above two adiabatic orbits point to $\vec{n}(\tau)$ and $-\vec{n}(\tau)$ at time τ, respectively. Considering the adiabatic orbit $|+,\tau\rangle$, the geometric potential of this orbit can be easily calculated as

$$\Delta_{mn} = \frac{\dot{\theta}\ddot{\phi}\sin\theta+2\dot{\theta}^2\dot{\phi}\cos\theta+\dot{\phi}^3\sin^2\theta\cos\theta-\dot{\phi}\ddot{\theta}\sin\theta}{\dot{\theta}^2+\left(\dot{\phi}\sin\theta\right)^2}. \tag{7}$$

As a comparison, we will calculate the geodesic curvature of the spherical curve $\vec{r}(\tau) = \vec{n}(\tau)$.

$$\begin{aligned}\rho &= \left(\vec{r}\times\frac{d\vec{r}}{ds}\right)\cdot\frac{d^2\vec{r}}{ds^2} \\ &= \frac{\dot{\theta}\ddot{\phi}\sin\theta + 2\dot{\theta}^2\dot{\phi}\cos\theta + \dot{\phi}^3\sin^2\theta\cos\theta - \dot{\phi}\ddot{\theta}\sin\theta}{\left(\sqrt{\dot{\theta}^2 + \left(\dot{\phi}\sin\theta\right)^2}\right)^3}, \quad (8)\end{aligned}$$

where curve element $ds = \left|d\vec{r}\right| = \sqrt{\dot{\theta} + \left(\dot{\phi}\sin\theta\right)^2}d\tau$. Then we get

$$\Delta_{mn} = \rho\frac{ds}{d\tau}. \quad (9)$$

Same result will be obtained in the case of adiabatic orbit $|-,t\rangle$ with corresponding spherical curve $\vec{r}(t) = -\vec{n}(t)$. This result shows a differential geometric property of the geometric potential. Besides, if we integrate the geometric potential over a close smooth curve we will obtain the difference of Berry phase between different adiabatic orbits

$$\begin{aligned}\oint\Delta_{mn}d\tau &= \arg\langle n|\dot{m}\rangle\,|_0^T + i\left(\oint\langle m|\,\dot{m}\rangle\,d\tau - \oint\langle n|\,\dot{n}\rangle\,d\tau\right) \\ &= i\left(\oint\langle m|\,\dot{m}\rangle\,d\tau - \oint\langle n|\,\dot{n}\rangle\,d\tau\right), \quad (10)\end{aligned}$$

which shows that the geometric potential also holds an integral geometric property.

In the following part, we will present some examples to show the significant effects caused by the geometric potential on the quantum adiabatic approximation. Let us study a modification of the model investigated in ref.[16]. The Hamiltonian is given as below

$$H(\tau) = \eta\sigma_z + \xi\left[\sigma_x\cos\left(2K\eta\tau\right) + \sigma_y\sin\left(2K\eta\tau\right)\right], \quad (11)$$

where $\eta > 0$, $\xi > 0$ and K are all constant parameters. For this kind of Hamiltonian Eq.(3) or Eq.(4) is a sufficient criteria for adiabatic approximation[17]. Choosing appropriate phases, the two adiabatic orbits can be written in following form

$$\begin{cases}|+,\tau\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{2iK\eta\tau}\sin\left(\frac{\theta}{2}\right)|1\rangle \\ |-,\tau\rangle = \sin\left(\frac{\theta}{2}\right)|0\rangle - e^{2iK\eta\tau}\cos\left(\frac{\theta}{2}\right)|1\rangle\end{cases}, \quad (12)$$

where $\cos\theta = \eta/\sqrt{\eta^2+\xi^2}$. Consider adiabatic orbit $|+,\tau\rangle$, we can calculate the geometric potential $\Delta_{+-} = 2K\eta\cos\theta$. It is easy to obtain the expression of the our adiabatic condition

$$\sqrt{\eta^2+\xi^2} - K\eta\cos\theta \gg K\eta\sin\theta. \quad (13)$$

Suppose the initial state of the system is $|+,0\rangle$, evolution states or *dynamic evolution orbit* reads

$$|\Psi(\tau)\rangle = e^{-iK\eta\sigma_z\tau}e^{-i((1-K)\eta\sigma_z+\xi\sigma_x)\tau}\,|+,0\,\rangle. \quad (14)$$

We can calculate the fidelity between the dynamic evolution orbit and the adiabatic orbit at time τ

$$\begin{aligned}F(\tau) &= |\langle+,\tau|\,U(\tau,0)\,|+,0\rangle| \\ &= \sqrt{\cos^2(A\tau) + \sin^2(A\tau)\left[\frac{(1-K)\eta\cos\theta + \xi\sin\theta}{A}\right]^2},\end{aligned}$$

where $A = \sqrt{(1-K)^2\eta^2 + \xi^2}$ is also a constant parameter.

If $K < 0$, both the traditional adiabatic condition and our condition guarantee the validity of the adiabatic approximation. If $K > 0$, there are two cases to which should be paid special attentions.

For the first case, we may choose $\eta \gg \xi$ and $K \simeq 1$, then the traditional condition is satisfied but our condition is not. Meanwhile, the fidelity $F(\tau) \approx \sqrt{1-\cos^2\theta\sin^2(A\tau)} \nrightarrow 1$ when τ is not too small. Thus, even though the traditional condition is satisfied and we might regard the system as slowly changing one, the quantum adiabatic approximation may be unfaithful description of the system because of the effect of the geometric potential. Fig.1 shows both the trajectory of polarization vectors of the dynamic evolution orbit and the adiabatic orbit on Bloch sphere surface when $K = 1$, $\eta = 1$ and $\xi = 0.1$. In the remain part of this paper, we will not distinguish state and its polarization vector and call just the former as evolution orbit and the latter as adiabatic orbit for simplicity.

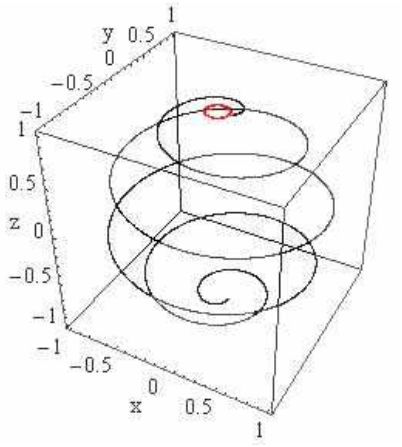

FIG. 1: evolution orbit(the black one) will be far away from adiabatic orbit(the red one) after several cycles of Hamiltonian

For the second case, we choose $\eta \gg \xi$ but $K \gg 1$. In this case the geometric potential is much larger than the difference of the instantaneous energy eigenvalues, and the our adiabatic condition is satisfied while the traditional one is not. Now we have $F(\tau) \approx \sqrt{1-\sin^2\theta\sin^2(A\tau)} \approx 1$. Therefore, the geometric potential can help to guarantee the validity of the adiabatic approximation despite the difference of energy eigenvalues is too small to satisfy the traditional condition. Fig.2 shows evolution orbit and adiabatic orbit for $K = 10$, $\eta = 1$ and $\xi = 0.1$. Fig.3 shows details after one cycle of

Hamiltonian and Fig.4 shows details after several cycles of Hamiltonian.

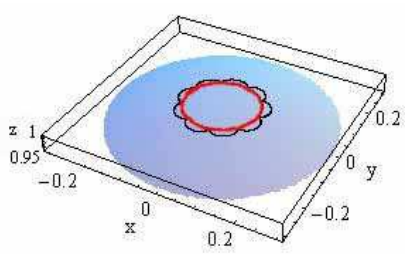

FIG. 2: evolution orbit and adiabatic orbit

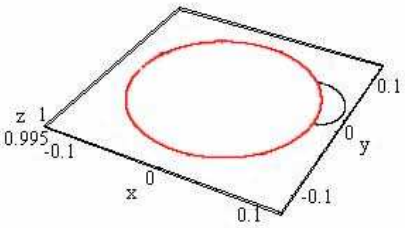

FIG. 3: Details of evolution orbit(the black line) and adiabatic orbit(red line) after one cycle of Hamiltonian

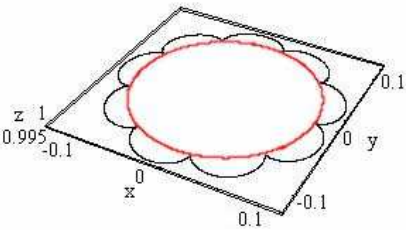

FIG. 4: Details of evolution orbit(the black line) and adiabatic orbit(red line) after many cycles of Hamiltonian

The lower bound of the fidelity $F(\tau)$ is $|((1-K)\eta\cos\theta+\xi\sin\theta)/A|$. If $K \gg 1$, the lower bound of fidelity can be approximated to be $\cos\theta$. The difference of the two adiabatic orbit's Berry phase is $2K\eta T\cos\theta = 2\pi\cos\theta$, where the T is the cycle period of the Hamiltonian. So we can conclude that larger the difference of the different adiabatic orbits' Berry phase is, more precise the quantum adiabatic approximation will be. And the conclusion is always correct in cases that the difference of the system's energy eigenvalues is small and geometric potential itself guarantees the validity of the adiabatic approximation.

At last, we will show a counterintuitive example. The Hamiltonian is given as below

$$\begin{cases} H = \vec{C}(\tau)\cdot\vec{\sigma}/2, \\ \vec{C}(\tau) = f(\tau)\vec{n}(\tau) + \vec{m}(\tau) \end{cases}, \tag{15}$$

where $\vec{n}(\tau) = (\sin\theta(\tau)\cos\phi(\tau), \sin\theta(\tau)\sin\phi(\tau), \cos\theta(\tau))$ and $\vec{m}(\tau) = \left(\dot{\theta}(\tau)\sin\phi(\tau), -\dot{\theta}(\tau)\cos\phi(\tau), \dot{\phi}(\tau)\right)$. Set the initial state be the eigenstate of the above Hamiltonian at initial time, it is easy to find out that if $\theta(0) = \dot{\theta}(0) = 0$, the evolution orbits of the given Hamiltonian read

$$\begin{cases} |\psi_+(\tau)\rangle = e^{i\int_0^\tau f(\lambda)d\lambda/2}\left(\cos\frac{\theta(\tau)}{2}|0\rangle + e^{i\phi(\tau)}\sin\frac{\theta(\tau)}{2}|1\rangle\right) \\ |\psi_-(\tau)\rangle = e^{-i\int_0^\tau f(\lambda)d\lambda/2}\left(\sin\frac{\theta(\tau)}{2}|0\rangle - e^{i\phi(\tau)}\cos\frac{\theta(\tau)}{2}|1\rangle\right) \end{cases}. \tag{16}$$

We choose $\varphi(\tau) = 5\tau + 0.15\sin[20\tau]$, $\theta(\tau) = \tau^{1.1}/50\pi$, and $\phi(\tau) = 0.2\tau$, evolution orbit and adiabatic orbit on Bloch sphere surface from time $\tau = 0$ to $\tau = 90\pi$ are shown in Fig.5 and Fig.6 respectively. We can see the adiabatic orbit is

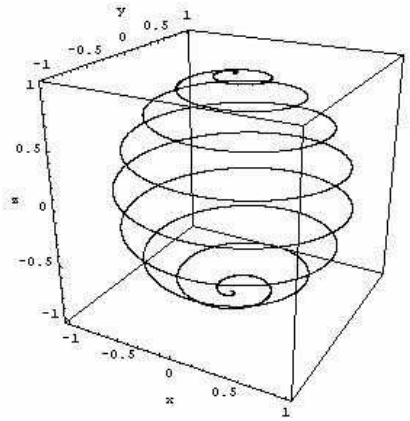

FIG. 5: Evolution orbit from $\tau = 0$ to $\tau = 90\pi$

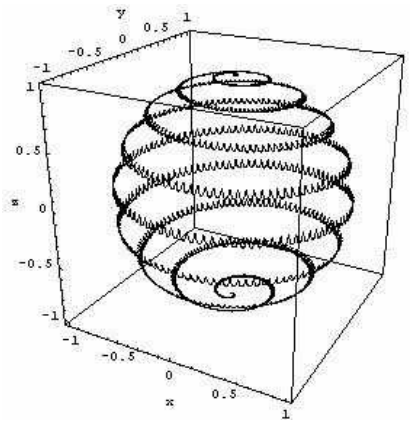

FIG. 6: Adiabatic orbit from $\tau = 0$ to $\tau = 90\pi$

a more complicated curve on Bloch sphere than the evolution orbit while they always hold a high fidelity $F \simeq 1$ during time $\tau = 0$ to $\tau = 90\pi$. It may be of some interests as it is a little

different from the common opinion about adiabatic approximation process.

In this paper we show the differential and integral geometric properties of the geometric potential presented in our recent paper , and then we discusses its effects on quantum adiabatic approximation. From traditional opinion, the difference between instantaneous energy eigenvalues $E_m(\tau) - E_n(\tau)$ represent the time-dependent quantum system's internal characteristic frequency. Furthermore, the existence of geometric potential suggests that the description of the time-dependent system's evolution might be more precise and more appropriate if we replace the difference of the systems' instantaneous energy eigenvalues by $E_m(\tau) - E_n(\tau) + \Delta_{mn}$. It seems to be a pity that Δ_{mn} does not satisfy the Rydberg-Ritz Combination Principle(RCP) because of the existence of the term $d \arg \langle n \mid \dot{m} \rangle / d\tau$. Moreover, when the instantaneous eigenstate does not satisfy the time-dependent Schrödinger equation, it is not a physical state, so RCP are not necessary to be satisfied. If $\langle n \mid \dot{m} \rangle = 0, \forall n \neq m$, the adiabatic orbit is exactly the dynamic evolution orbit and this orbit become physical states, RCP are satisfied automatically. What surprises us is that Δ_{mn} in our adiabatic condition relates closely to the geometric property of the Hamiltonian's parametric space and the adiabatic orbits. It is quite clear that non-trival geometric properties will more or less affect the evolution process as long as the Hamiltonian varies with time.

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* Electronic address: zmesson@mail.ustc.edu.cn

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